Torsion 12 [!#1;R2;r5:1]@[CX4;R1;r5:2]@;-[CX4;R1;r5:3]@[!#1;R2;r5:4] 0.035 0.030 10° Bin 0.025 **Binned Counts** per 0.020 -Trig. Fit Probability **ETKDG Fit** 0.015 -0.010 -0.005 -0.000 60 120 180 Torsion (°)